

«beta»-Phellandrene

Other names:	3-Isopropyl-6-methylenecyclohexene 3-methylene-6-(1-methylethenyl)-cyclohexane 3-methylene-6-(1-methylethenyl)-cyclohexane («beta»-phellandrene) 3-methylene-6-(1-methylethenyl)-cyclohexane (Â«betaÂ»-phellandrene) Cyclohexene, 3-methylene-6-(1-methylethyl)- Phellandrene, «beta» Phellandrene, Â«betaÂ» beta-Phellandrene p-Mentha-1(7),2-diene
Inchi:	InChI=1S/C10H16/c1-8(2)10-6-4-9(3)5-7-10/h4,6,8,10H,3,5,7H2,1-2H3
InchiKey:	LFJQCDVYDGGFCH-UHFFFAOYSA-N
Formula:	C10H16
SMILES:	C=C1C=CC(C(C)C)CC1
Mol. weight [g/mol]:	136.23
CAS:	555-10-2

Physical Properties

Property code	Value	Unit	Source
gf	138.37	kJ/mol	Joback Method
hf	-58.67	kJ/mol	Joback Method
hfus	10.03	kJ/mol	Joback Method
hvap	38.35	kJ/mol	Joback Method
log10ws	-3.13		Crippen Method
logp	3.165		Crippen Method
mcvol	132.300	ml/mol	McGowan Method
pc	2741.15	kPa	Joback Method
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ripol	1215.00		NIST Webbook
tb	445.63	K	Joback Method
tc	651.00	K	Joback Method
tf	209.28	K	Joback Method
vc	0.492	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	361.70	J/molxK	651.00	Joback Method
cpg	270.36	J/molxK	445.63	Joback Method
cpg	287.65	J/molxK	479.86	Joback Method
cpg	304.09	J/molxK	514.09	Joback Method
cpg	319.70	J/molxK	548.32	Joback Method
cpg	334.48	J/molxK	582.55	Joback Method
cpg	348.47	J/molxK	616.77	Joback Method
dvisc	0.0002490	Paxs	445.63	Joback Method
dvisc	0.0047798	Paxs	209.28	Joback Method
dvisc	0.0019776	Paxs	248.67	Joback Method
dvisc	0.0010415	Paxs	288.06	Joback Method
dvisc	0.0006401	Paxs	327.45	Joback Method
dvisc	0.0004367	Paxs	366.85	Joback Method
dvisc	0.0003209	Paxs	406.24	Joback Method
hvapt	47.70	kJ/mol	333.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.35838e+01
Coeff. B	-3.62351e+03
Coeff. C	-5.45410e+01
Temperature range (K), min.	327.06
Temperature range (K), max.	492.57

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C555102&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices

tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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